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ON SIMPLEX SHAPE MEASURES WITH EXTENSION FOR ANISOTROPIC MESHES

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ABSTRACT: This paper surveys and analyses several simplex shape measures documented in the literature and used for mesh adaptation and mesh optimization. The paper first summarizes important properties of simplices and their degeneracies in Euclidean space. Each shape measure is then defined and validated with respect to a proposed shape measure validity criterion. Extensions to Riemannian spaces are proposed in order to deal with anisotropic meshes. A visualization scheme is also presented, which helps compare shape measures to one another.

KEY WORDS: triangle, tetrahedron, simplex shape measures, unstructured grid, mesh optimization, anisotropy, metric.

Introduction

Shape measures provide an effective quantitative mean of evaluating the quality of the elements in a mesh which is of great relevance in mesh adaptation and mesh optimization. Still, while most serious work in the field of mesh adaptation directly make use of shape measures [19, 27, 28, 33], very little work has been devoted to the actual comparison of shape measures, with the notable exceptions of Liu and Joe [23, 24, 25, 26] who have thoroughly analyzed selected shape measures, early work by Parthasarathy *et al.* [30], and recent work by Georges and Frey [19, 16].

While these published works present some of the standard shape measures in current use, new shape measures steadily appear in recent literature for which no analysis is available. Furthermore, no classification scheme has been proposed, and fitness of new measures is often not assessed.

This paper aims to survey a wider range of shape measures in general use, to define validity criteria for those measures and to classify them in broad

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categories, beginning with valid shape measures. The paper also addresses issues regarding the use of shape measures in non-Euclidean spaces in order to be applicable to anisotropic meshes. Extensions are thus provided for the use of shape measures in Riemannian spaces.

The first section of the paper summarizes important properties of simplices and introduces a classification of simplex degeneracies in 2 and 3 dimensions. The next section introduces shape measures validity criteria, presents a wide range of shape measures, and explains how to use them in a Riemannian space which enables their use for anisotropic meshes. The third section presents a visualization scheme that helps analyze and compare shape measures to one another. Implications of the choice of a shape measure into a mesh optimization process is both theoretically and practically explored. Conclusions are drawn on the pertinence of developing new shape measures or choosing one among the currently existing ones.

1 Simplices

This section summarizes some well known properties of simplices, and introduces some often neglected notions about simplex degeneracies that will be used as foundations for the classification of shape measures and their comparison.

1.1 Definition of a Simplex

A *simplex*, in a space of dimension d, is the convex hull of $d+1$ vertices, and represents the simplest element that can be used to discretize space in that dimension. In practice, a simplex is a triangle in two dimensions and a tetrahedron in three dimensions. A more general discussion on simplices can be found in [16].

1.2 Regular Simplices

A regular simplex is an equilateral triangle in two dimensions and an equilateral tetrahedron in three dimensions. Equilaterality implies that all edges have the same length, which relies on the notion of distance, or in a general sense, on the notion of a metric. By changing the metric tensor used in the metric, it is possible to generate anisotropic meshes. In this way, anisotropic meshes are made up of equilateral elements when measured using the appropriate metric tensor.

Appendices B and C summarize a number of useful formulae that relate properties of triangles and tetrahedra to their edge lengths. These relations will be used in section 2 to define the simplex shape measures in Euclidean space. Possible extensions to Riemannian spaces will also be discussed.

1.3 Degenerate Simplices

A simplex is *degenerate* if its vertices are all included in a subspace. That is, a d-simplex is degenerate if its $d+1$ vertices do not span space $\mathbb{R}^d$. This means that a triangle is degenerate when the three vertices are collinear, or *a fortiori* when they collapsed into a single point. A tetrahedron is degenerate when its four vertices are coplanar, or *a fortiori* when they are collinear or collapsed. In practice, degeneration detection is replaced by a test on area or volume. A triangle is degenerate if its area vanishes, and a tetrahedron is degenerate if its volume vanishes.

The most systematic way of classifying simplex degeneracies is not to consider the process that leads to the degeneracy but rather the final configuration of the degenerate simplex. In order to systematically classify simplex degeneracies, the following notation, inspired from astronomical atlases, is used : the four symbols , , and will respectively be used to denote vertices of multiplicity one, two, three and four.

Tables 1 to 3 presents simplex degeneracies. For each type of degeneracy, a name inspired from the literature (mostly Bern *et al.* [2, 3]) is used when available, and degenerate cases not yet identified are given distinctive names.

Table 1: The three degeneracies of triangle: *NDE* is the number of degenerate edges, and r_K is the circumradius limit.

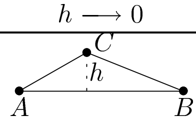
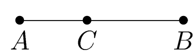
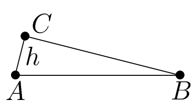
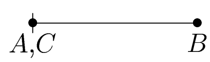
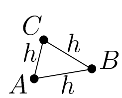
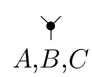
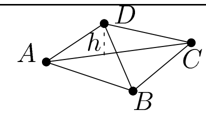
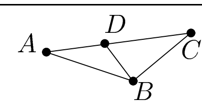
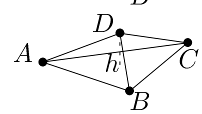
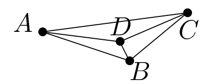
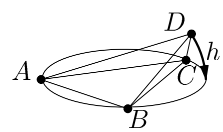
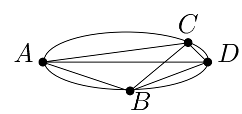
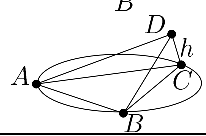
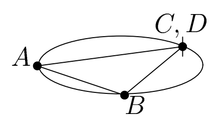
Name	$h \longrightarrow 0$	$h = 0$	*NDE*	r_K
Cap			0	∞
Needle			1	$\frac{h_{max}}{2}$
Big Crunch			3	0

Table 1 lists the three degenerate cases for the triangle. Each case is illustrated before and at degeneracy, and for each case, the number of short edges and the final circumcircle radius are listed. These informations are central to the analysis of shape measures, as they are often used to detect degenerate cases, and are thus included in the computation of various shape measures. In the *Needle* degeneration case, the listed circumcircle radius $h_{max}/2$ corresponds the half-length of the two non-degerate edges of the degenerate triangle.

Table 2 presents the four types of planar tetrahedral degeneracies and Table 3 presents the five types of linear degeneracies, and the punctual tetrahedral degeneracy.

Table 2: The four planar degeneracies of tetrahedron: NDE is the number of degenerate edges, $\triangle$ is the type of degenerate triangular faces (c =cap, n =needle), r_K is the limit of the circumsphere radius and r_{ABC} is the circumcircle radius of triangle ABC.

Name	$h \longrightarrow 0$	$h = 0$	NDE	$\triangle$	r_K
Fin			0	$1c$	∞
Cap			0	0	∞
Sliver			0	0	r_{ABC} or ∞
Wedge			1	$2n$	r_{ABC}

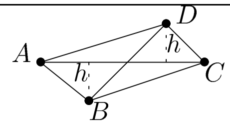
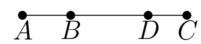
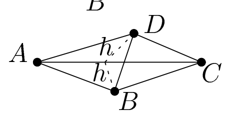
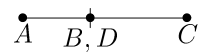
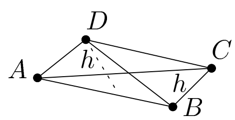
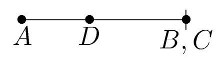
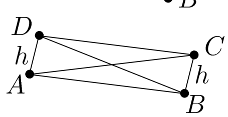
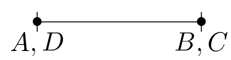
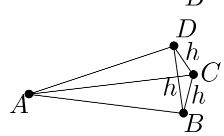
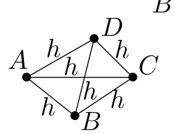
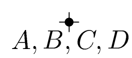
2 Shape Measures of Simplices

The concept of shape measure is widely used in the mesh adaptation literature, but while the use of this notion is quite spread, few papers actually define and compare various shape measures one to another. In this regard, papers by Liu and Joe [23, 25, 26], and especially reference [24] stand as landmark work on the topic. Other reviews of tetrahedron shape measures appear as well in George and Borouchaki [19] and Parthasarathy *et al.* [30]. The underlying idea behind all simplex shape measures is to define a way to quantify the shape of a simplex. In particular, this quantity should be optimal for the regular simplex and it should be sensitive to all simplex degeneracies. There are so many simplex shape measures in the literature that we suggest the following global definition, introduced in Dompierre *et al.* [11] and derived form Liu and Joe [24]:

Definition 2.1. *A* **simplex shape measure** *is a continuous function that evaluates the shape of a simplex. It must be invariant under translation, rotation, reflection and uniform scaling of the simplex. It must be maximum for the regular simplex and it must be minimum for all degenerate simplices. For the ease of comparison, it should be scaled to the interval* $[0, 1]$*, and be* 1 *for the regular simplex and* 0 *for a degenerate simplex.*

In this definition, the invariance by translation, rotation and reflection

Table 3: The five linear degeneracies of tetrahedron and the punctual degeneracy: *NDE* is the number of degenerate edges, $\triangle$ is the type of degenerate triangular faces (c =cap, n =needle, BC=Big Crunch), r_K is the limit of the circumsphere radius.

Name	$h \longrightarrow 0$	$h = 0$	*NDE*	$\triangle$	r_K
Crystal			0	$4c$	∞
Spindle			1	$2c$ $2n$	∞
Splitter			1	$2c$ $2n$	∞
Slat			2	$4n$	$\frac{h_{max}}{2}$
Needle			3	$3n$ $1BC$	$\frac{h_{max}}{2}$
Big Crunch			6	$4BC$	0

makes the measure independent from any coordinate system. The invariance by uniform scaling of the simplex makes it independent from any measurement units. This is not considered to be a degenerate tetrahedron until the volume as actually reached zero. Also under this definition, continuity requirements are to ensure that if a simplex is close to the regular simplex, then the simplex shape measure should be close to 1. Conversely, if a simplex is close to being degenerate, then the simplex shape measure should be close to 0. Any simplex shape measure that satisfies Definition 2.1 is a *valid* simplex shape measure, and any criterion considered as a simplex shape measure but that does not satisfy Definition 2.1 is said to be an *invalid* simplex shape measure.

When the area of a triangle or the volume of the tetrahedron is negative, the simplex is more than degenerate, it is inverted. In this case, some simplex shape measures return a negative number, and some others return a positive number because, for example, they depend on the square of the area or of the volume. Due to the invariance by reflection, any valid simplex shape measure returns a positive number. Simplex shape measures should not be used to determine whether a simplex is inverted. Rather, if a mesh contains inverted simplices, the mesh optimizer should try to remove them by optimizing the volume of the tetrahedra or the area of the triangles, by minimizing the sum of the absolute value of the volumes or of the areas as proposed by Coupez [10]. In the context of inverted simplices, the shape of the inverted simplex is irrelevant, what matters is its size.

A review of simplex shape measures is presented in the following subsections. The shape measures are grouped in broad categories according to the fundamental measures involved in their computation. Each shape measure is classified as valid or invalid according to Definition 2.1. A short discussion follows to extend these measures to the case of anisotropic meshes.

2.1 Linear Transformation Based Shape Measures

Many authors introduce shape criteria constructed from the matrix involved in the linear transformation of a simplex K to a regular reference simplex. While the choice of the defining parameters of the reference simplex (in terms of vertex numbering, coordinates, etc.) is somewhat arbitrary and impacts on the transformation matrix N, the product $N^T N$ does not depend of those parameters. Indeed, all these matrices induce the same metric tensor $\mathcal{M}_K$ (see Eq. A.4), which transforms simplex K into an equilateral simplex. This metric tensor is uniquely defined, and can also be determined by solving a linear system of equations that expresses the constraint whereby each edge of the simplex K is brought to unit length.

Liu and Joe [24] have defined the transformation matrix M in a simplex K of a regular simplex with the same size (same area for triangles and same volume for tetrahedra). The *mean ratio* shape measure η can be written as:

$$\eta = \frac{\left(\prod_{i=1}^{d} \lambda_i\right)^{1/d}}{\frac{1}{d}\sum_{i=1}^{d} \lambda_i} = \begin{cases} \dfrac{2\,(\lambda_1\lambda_2)^{1/2}}{\lambda_1+\lambda_2} = \dfrac{4\sqrt{3}\,S_K}{\sum\limits_{1\le i<j\le 3} L_{ij}^2} & \text{in 2 D,} \\[2ex] \dfrac{3\,(\lambda_1\lambda_2\lambda_3)^{1/3}}{\lambda_1+\lambda_2+\lambda_3} = \dfrac{12\sqrt[3]{9V_K^2}}{\sum\limits_{1\le i<j\le 4} L_{ij}^2} & \text{in 3 D.} \end{cases} \tag{2.1}$$

where the λ_i, $i = 1, \ldots, d$ are the eigenvalues of the matrix $M^T M$ in dimension d. Notations are detailed in Appendices A, B and C.

Formaggia and Perotto [13] introduce another linear application N and define the *stretching factor* of simplex K as the ratio of the largest to the smallest eigenvalue of N^{-1}. This stretching factor is also the square root of the *condition number* of matrix $\mathcal{M}_K$. The condition number κ of a simplex is then defined as the inverse of the condition number of matrix $\mathcal{M}_K$. κ is a shape measure which is expressed as

$$\kappa = \frac{\min\limits_i \lambda_i}{\max\limits_i \lambda_i} = \frac{\lambda_1}{\lambda_d}, \tag{2.2}$$

if the eigenvalues are sorted in increasing order.

Knupp et Freitag [22, 14] have introduced another shape measure, also called the *condition number*, based on a composition of linear applications that first transforms a simplex K into a right angled reference element (such as used in finite element analysis) and then transforms this right angled element into an equilateral simplex of unit edge length. The transformation matrix is denoted $S = AW^{-1}$ and is the inverse of the transformations described above, going from reference space to real space. The condition number of simplex K is defined as the product of Frobenius' norm of the matrix and of its inverse. Frobenius' matrix norm is defined as

$$\|S\| = \left(\mathrm{tr}(S^T S)\right)^{1/2}.$$

The matrix $S^T S$ involved in the norm of S is the inverse of the metric tensor, ie $\mathcal{M}_K^{-1}$. It is proven in [14] that the inverse of the condition number, scaled by the space dimension,

$$\widetilde{\kappa} = \frac{d}{\|S\| \, \|S^{-1}\|} \tag{2.3}$$

is a shape measure $\widetilde{\kappa}$ according to Definition 2.1.

2.2 The Radius Ratio

The radius ratio ρ of a simplex K is defined to be $\rho = d\rho_K / r_K$ where ρ_K and r_K are the inradius and circumradius of K, respectively, and d is the dimension of the space. Using the Eqs. (B.1) and (C.2) of ρ_K and r_K in two and three dimensions, the radius ratio is written as

$$\rho = d\frac{\rho_K}{r_K} = \begin{cases} \dfrac{8S_K^2}{p_K \, L_{12} \, L_{13} \, L_{23}} & \text{in 2 D,} \\ \dfrac{216V^2}{\sqrt{(a+b+c)(a+b-c)(a+c-b)(b+c-a)} \sum_{i=1}^{4} S_i} & \text{in 3 D,} \end{cases} \tag{2.4}$$

where a, b and c are the products of opposite edge lengths of a tetrahedron K.

2.3 The Minimum of the Solid Angles

A mesh is a Delaunay mesh if the circumsphere of each element does not contain any other vertex of the mesh. In two dimensions, the Delaunay property is equivalent to maximize the minimum of the angles of the triangles of the mesh, called the max–min angle criterion. It was therefore natural to use the minimum of the angles of a triangle as a shape measure. This shape measure in two dimensions will yield a mesh satisfying the Delaunay criterion.

In three dimensions, Delaunay meshes do not generally satisfy the max–min angle criterion [32]. Remember that a mesh containing badly shaped tetrahedra like the sliver in Table 2 can pass the Delaunay criterion. A simplex shape measure based on the minimum of the solid angles θ_{min} will result in meshes of better quality than Delaunay meshes having some sliver elements.

The solid angle θ_i at the vertex P_i of a tetrahedron K is defined to be the surface area formed by projecting each point of the face not containing P_i to the unit sphere centered at P_i.

The *minimum of the solid angles* simplex shape measure is defined as

$$\theta_{min} = \alpha^{-1} \min_{1 \le i \le n+1} \theta_i, \tag{2.5}$$

where θ_i is given by Eq. (B.3) in two dimensions; θ_i is given by Eq. (C.4) in three dimensions; $\alpha = \pi/3 \simeq 1.047$ is the value of the three solid angles of the regular triangle and $\alpha = 6 \arcsin\left(\sqrt{3}/3\right) - \pi \simeq 0.551$ is the value of the four solid angles of the regular tetrahedron.

This measure is sensitive either to narrow and to large solid angles. In two dimensions, the maximum of the solid angles in a triangle is π, the sum of the solid angles of a triangle is π and a large solid angle near π implies that the triangle has also small solid angles. In three dimensions, the area of a unit sphere is 4π, the maximum of the solid angles for a positive tetrahedron is 2π in the case of a flat tetrahedron where a vertex sees half of the space. The solid angle at the corner of a right-angled tetrahedron is $\pi/2$. It is shown in Gaddum [17] that $0 \le \sum_{i=1}^{4} \theta_i \le 2\pi$. Therefore, a large solid angle near 2π for K implies that K has small solid angles.

The evaluation of the expression $\theta_i = 2 \arcsin(\cdot)$ is always in the interval $[0,\ \pi]$. It means that the Eq. (C.4) can be only used to measure solid angles less or equal to π. So the maximum solid angle of a tetrahedron can wrongly be evaluated using Eq. (C.4). However, the minimum of the solid angles is not affected. Let $\theta_1 \le \theta_2 \le \theta_3 \le \theta_4$. Since $0 \le \sum_{i=1}^{4} \theta_i \le 2\pi$, only θ_4 may be larger than π. The computation with Eq. (C.4) of θ_4 returns $\widetilde{\theta}_4 = 2\pi - \theta_4$. Substituting θ_4 by $2\pi - \widetilde{\theta}_4$ in $\sum_{i=1}^{4} \theta_i \le 2\pi$ gives $\theta_1 + \theta_2 + \theta_3 \le \widetilde{\theta}_4$. So, θ_1 which is lower or equal to θ_2 and θ_3 is also lower or equal to $\widetilde{\theta}_4$. The conclusion is that even if the Eq. (C.4) does not return the correct value for a solid angle greater than π, it does not affect the tetrahedron shape measure (2.5) based on the minimum of the solid angles. An equivalent deduction can be done in two dimensions.

Instead of computing the $\arcsin(\cdot)$ in Eq. (B.3) and (C.4), from a computational point of view, a cheaper simplex shape measure is used in [24]

$$\sigma_{min} = \beta^{-1} \min_{1 \le i \le n+1} \sigma_i, \tag{2.6}$$

where $\sigma_i = \sin(\theta_i)$ in two dimensions; $\sigma_i = \sin(\theta_i/2)$ in three dimensions; $\beta = \sin(\alpha) = \sqrt{3}/2 \simeq 0.866$ is the value of σ_i for the three solid angles of the regular triangle; and $\beta = \sin(\alpha/2) = \sqrt{6}/9 \simeq 0.272$ is the value of σ_i for the four solid angles of the regular tetrahedron.

2.4 The Interpolation Error Coefficient

In finite element analysis there are theorems [34] that bound the interpolation error of a function over a finite element with a coefficient multiplied by the semi-norm of the function. This coefficient is something like D_K/ϱ_K where D_K is the diameter of the element K and ϱ_K is the roundness of the element K. The diameter of an element is the length of the greatest straight line inside the element. For a simplex, it is the longest edge. The roundness of an element is the diameter of the greatest sphere (circle in two dimensions) included in the element. For a simplex, it is twice the inradius. The diameter and the roundness are defined for simplicial and non simplicial elements but it is not necessarily easy to compute the diameter of the greatest sphere included in an hexahedron or a prism.

When a simplex K is degenerate or close to, the diameter D_K is large and the roundness ϱ_K is small, then the coefficient D_K/ϱ_K is a large value that indicates a large bound for the interpolation error. So, this coefficient can be used to measure the shape of a simplex K. (Note that a large bound for the interpolation error does not necessarily mean that the interpolation error is effectively large).

To be compatible with Definition 2.1 of the simplex shape measures and to avoid division by zero for degenerate simplices, the *interpolation error coefficient* simplex shape measure is defined using the inverse of the coefficient of the interpolation error. This simplex shape measure is named γ, according to publications from the GAMMA project (Génération Automatique de Maillages et Méthodes d'Adaptation) at the Institut National de Recherche en Informatique et en Automatique (INRIA), France [19, 7, 15, 18, 19].

$$\gamma = \begin{cases} 2\sqrt{3}\,\dfrac{\rho_K}{h_{max}} & \text{in 2 D,} \\ \dfrac{12}{\sqrt{6}}\,\dfrac{\rho_K}{h_{max}} & \text{in 3 D.} \end{cases} \tag{2.7}$$

2.5 The Minimum of the Dihedral Angles

The minimum of the dihedral angles is a tetrahedron shape measure that has no two-dimensional equivalent. The dihedral angle at an edge of a tetrahedron is the angle between the intersection of the two faces sharing this edge and a plane perpendicular to the edge. For a positive tetrahedron, the dihedral angle is bounded by zero and π. It is equal to π minus the angle between the normals of the faces.

$$\varphi_{min} = \alpha^{-1} \min_{1 \le i < j \le 4} \varphi_{ij} = \alpha^{-1} \min_{1 \le i < j \le 4} \left(\pi - \arccos\left(n_{ij1} \cdot n_{ij2}\right)\right), \tag{2.8}$$

where n_{ij1} and n_{ij2} are the two normals to the triangular faces adjacent to the edge ij and $\alpha = \pi - \arccos(-1/3) = 1.231$ is the value of the six dihedral angles of the regular tetrahedron. The minimum of the dihedral angles is sometimes used as a tetrahedron shape measure.

According to Definition 2.1 of a tetrahedron shape measure, the minimum of the dihedral angles φ_{min} is an *invalid* tetrahedron shape measure. The underlying problem with tetrahedron shape measures based on the dihedral angles is that they fail to detect some degenerate tetrahedra. Referring to Table 3, the smallest dihedral angle of the needle can be as large as $\frac{\pi}{3}$ and the largest dihedral angle as small as $\frac{\pi}{2}$. The spindle and the crystal can have a minimum dihedral angle close to $\frac{\pi}{3}$, with a maximum dihedral angle close to π.

2.6 The Edge Ratio

The edge ratio r of a simplex K is defined to be the ratio between the length of the shortest edge over the longest, i.e.,

$$r = h_{min}/h_{max}, \tag{2.9}$$

where h_{min} and h_{max} are defined by Eqs. (B.2) and (C.3).

According to Definition 2.1 of a simplex shape measure, the edge ratio r is an *invalid* simplex shape measure because it does not vanish for all degenerate simplices. In two dimensions, it can be as large as $\frac{1}{2}$ for the cap. In three dimensions, it can be as large as $\frac{\sqrt{2}}{2}$ for the sliver, $\frac{1}{2}$ for the fin, $\frac{\sqrt{3}}{3}$ for the cap and $\frac{1}{3}$ for the crystal.

2.7 The Delaunay Criterion as a Shape Measure

The Delaunay criterion can be used to connect vertices to built a simplicial mesh. As seen above in Sec. 2.3, using this criterion in two dimensions is strictly equivalent to reconnecting vertices regarding to the minimum of the angles shape measure.

Remarks must be made about three-dimensional meshes satisfying the Delaunay criterion. It is important to note that valid simplex shape measures will detect slivers. Since meshes that satisfy the Delaunay criterion can nevertheless contain slivers, satisfying the Delaunay criterion does not constitute a guarantee that a mesh does not contain degenerate tetrahedra, and in that respect, the Delaunay criterion by itself does not act as a valid shape measure.

2.8 Extension to Riemannian Spaces

All simplex shape measures have been presented here in the frame of the usual Euclidean space. In order to get anisotropic meshes, these measures are now extended to the context of a Riemannian space.

A metric tensor is a tensor representing the deformation of space equivalent to the size specification map. Appendix A summarizes notions about metrics used in this paper, and exhaustive discussions on the topic of metrics can be found in [12, 21, 20, 5, 8, 9, 6, 4] among many others; the first references being Vallet [36, 37], and the most complete being George and Borouchaki [19, 16].

A Riemannian metric is defined by a metric tensor field (see Appendix A) whose variations must be continuous. For meshing purpose, we assume smooth variations of the metric. With this assumption metric variations can be locally neglected resulting in a local uniform, eventually stretched, metric.

Practically, the metric tensor $\mathcal{M}(P)$ is averaged on a simplex into $\overline{\mathcal{M}}$ using a quadrature formula for each of its coefficients. This yields an Euclidean space that is not necessarily Cartesian (the tensor is not necessarily the identity matrix). Edge lengths are then computed using Eq. (A.2) with a uniform metric tensor. This simplifies in

$$L_{ij}^{\mathcal{M}} = \sqrt{(P_j - P_i)^T \, \overline{\mathcal{M}} \, (P_j - P_i)}. \tag{2.10}$$

Simplex measures are computed the same way using Eq. (A.5) where $\mathcal{M}$ is approximated by $\overline{\mathcal{M}}$. Hence, expressions for area of a triangle and volume of a tetrahedron in the local metric simplify into

$$S_K^{\mathcal{M}} = S_K \sqrt{\det(\overline{\mathcal{M}})}, \tag{2.11}$$

and

$$V_K^{\mathcal{M}} = V_K \sqrt{\det(\overline{\mathcal{M}})}. \tag{2.12}$$

The other simplex characteristics ρ_K, r_K, h_{min}, h_{max} and θ_i can now be approximated in the local metric using $L_{ij}^{\mathcal{M}}$, $S_K^{\mathcal{M}}$ and $V_K^{\mathcal{M}}$ in the approximate formulas given in Appendices B and C. Finally, simplex shape measures can be approximated in the Riemannian metric.

3 Comparison of Triangle Shape Measures

A method is presented that helps to visualize the behavior of the various shape measures. This method is used to compare and choose a shape measure for its simplicity and its regularity. The effect of the metric tensor stemming from the anisotropic mesh is also illustrated.

3.1 Visualization of Triangle Shape Measures

Vallet [37] introduced a way to visualize the shape measure of a triangle. Consider three vertices A, B and $C3$ lying on the xy-plane (Fig. 1 left). The vertex A is at coordinate $(0,\ \frac{1}{2})$, the vertex B is at coordinate $(0,\ \frac{-1}{2})$ and the vertex C, at coordinate $(x,\ y)$, is free to move in the half-plane $x \geq 0$.

At each location of vertex C, a given shape measure of the triangle ABC is evaluated which gives the three-dimensional plot of the shape measure shown in Fig. 1 on right. Using this method, Figs. 2 and 3 show the contour plot of each triangle shape measure introduced in Section 2. By examining these contour plots, it is easy to assess whether a triangle shape measure is valid according to the Definition 2.1: valid shape measures reach a maximum for the equilateral triangle at coordinate $(\frac{\sqrt{3}}{2},\ 0)$; a minimum has to be zero and must be reached on the y-axis where the three vertices of the triangle are collinear. Between these two extrema, the triangle shape measure must be a continuous function

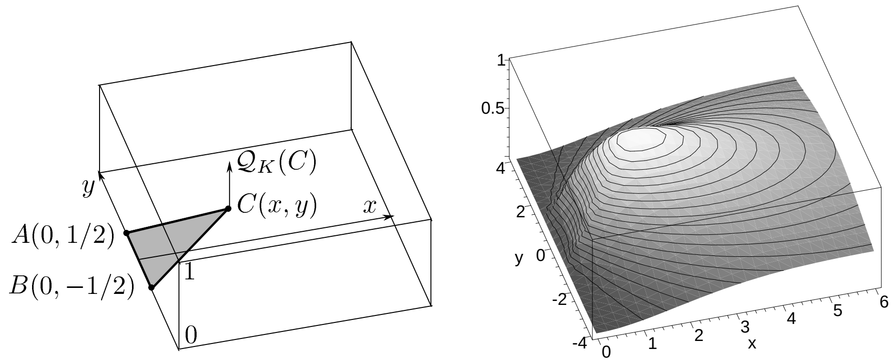


Figure 1: Definition of the location of the three vertices A, B and C of a triangle (left) to build the three-dimensional plot of the triangle shape measure (right).

with values between 0 and 1 exclusively. These plots show that the edge ratio is not a valid triangle shape measure (see Fig. 3 on right) because it does not vanish on the y-axis where the three vertices are collinear and the triangle is degenerate.

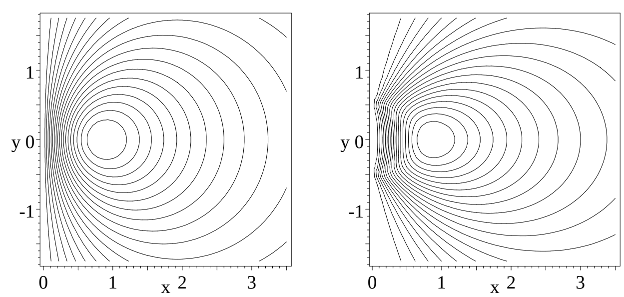


Figure 2: Contour plot of the mean ratio shape measure η (Eq. (2.1)) left, and of the radius ratio shape measure ρ (Eq. (2.4)) right.

3.2 Choice of a measure for mesh optimization

Analysis of Fig. 2 and 3 helps to determine which triangle shape measure is the most convenient to use for mesh optimization. Clearly, an invalid simplex shape measure is a bad choice because it will not detect degenerate simplices and may drive the mesh optimizer in a wrong direction. Note however that in the neighborhood of the regular triangle, the contour lines of all shape measures have a correct behavior. Even the triangle edge ratio measure r, plotted in

Fig. 3 on right will yield correct meshes as long as the mesh optimizer stays far away from degenerate triangles.

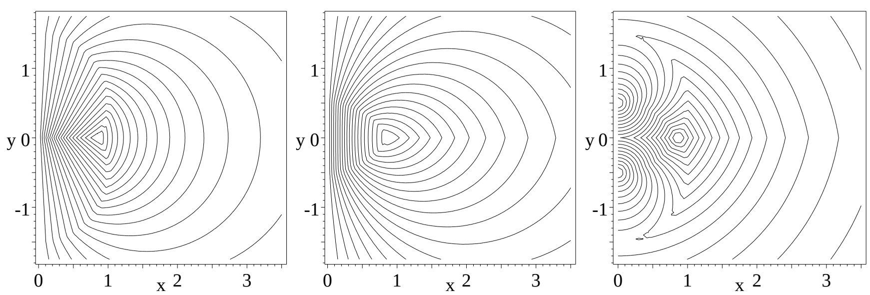


Figure 3: Contour plot of the minimum of solid angles shape measure θ_{min} (Eq. (2.5)) on left; of the interpolation error coefficient shape measure γ (Eq. (2.7)) in center and of the edge ratio measure r (Eq. (2.9)) on right.

All valid triangle shape measures plotted in Figs. 2 and 3 are continuous. Among them, ρ and η are derivable, but θ_{min} and γ are not derivable along curves because these measures use the minimum or maximum operator, which are not derivable. Non derivable simplex shape measures can be used for mesh optimization but convergence may be less efficient.

Another well known feature of optimization algorithms is that the convergence is easier and faster if the function to maximize is circular around the optimal point. Conversely, the convergence will be slower if the function to maximize has sharp ridges (or narrow valleys for minimization problems). Finally, consider that the simplex shape measure ρ evaluated with Eq. (2.4) is an undefined fraction for some degenerate simplices. Moreover, as proved in [1], contour plots drawing the mean ratio measure η are circles. The conclusion from these remarks is that the mean ratio η is the most convenient simplex shape measure for two dimensional mesh optimization. It is also the less expensive to evaluate numerically.

So, from a practical point of view, the mean ratio η is the most convenient triangle and tetrahedron shape measure to use in a mesh optimizer.

3.3 Visualization of anisotropic shape measure

The effect of the metric tensor on the contour plot of the shape measure can also be illustrated. Indeed, as presented in sections 1.2 and 2.8, the metric tensor takes into account the anisotropy required for the mesh. Thus, the metric tensor stores the information necessary to specify the stretching and the orientation of the simplex to build. If the metric tensor is constant, it induces an Euclidean space that modifies the optimal position of the third vertex.

Figure 4 presents the contour plot of the two dimensional η shape measure for three different metric tensors. The η shape measure being the ratio of the area of the triangle over the sum of square of the length of the edges of the triangle(equation (2.1)). In order to take into account the different metric tensors, the area of the triangle in the metric space is computed using equation (A.5) and the length of the edges in the metric space are computed using equation (A.2). For a constant metric tensor, equation (A.2) can be simplified to equation (2.10) and the area of the triangle in the metric space can be written as a function of the length of its edges by using Héron's formula (B.4).

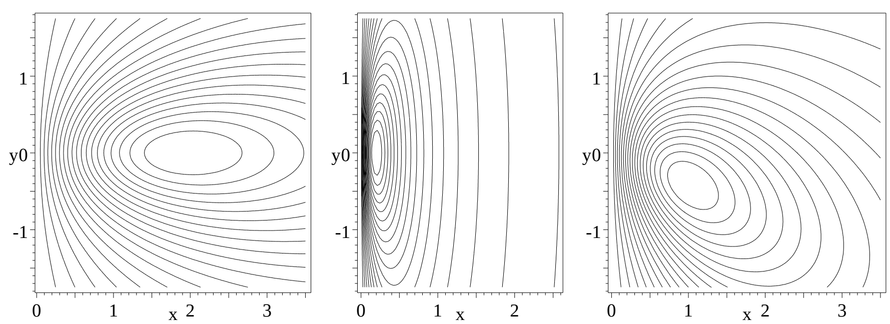


Figure 4: Contour lines of the η shape measure, based on the average ratio (equation (2.1)), for three constant metric tensors.

In Fig. 4, the metric tensor $\mathcal{M}$, is a positive definite symmetric tensor that is equal to $m_{11} = 0.2$, $m_{12} = 0$ and $m_{22} = 1$ for the figure on the left, $m_{11} = 20$, $m_{12} = 0$ and $m_{22} = 1$ for the figure in the middle and $m_{11} = 0.9$, $m_{12} = 0.4$ and $m_{22} = 1$ for the figure on the right. In comparison, Fig.2 on the right is nothing more than a representation of the η shape measure for which the metric tensor is the identity matrix. In these four graphs, degeneracies appear when the vertices are collinear and is independent of the metric tensor. However, the optimal position of the third vertex of the simplex depends on the value of the metric tensor used. Moreover, the contour lines of the η shape measure, that are circles for the identity matrix, now become ellipses in the general case.

4 Implications for Mesh Optimization

For mesh optimization, all shape measures are more or less interchangeable, despite their differences. To illustrate the similarity of various shape measures, Fig. 5 shows a superposition of contour plots drawn previously.

This similarity can be formalized by the notion of equivalence between shape measures.

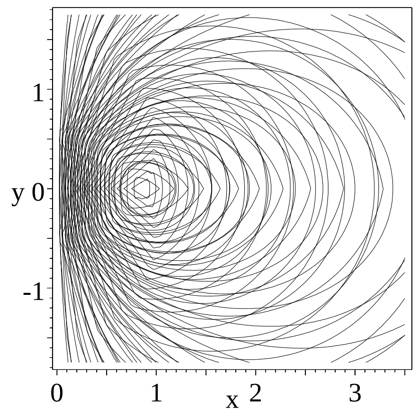


Figure 5: Superposition of the contour plot of the triangle shape measure η (Eq. (2.1)), ρ (Eq. (2.4)), θ_{min} (Eq. (2.5)) and γ (Eq. (2.7)).

4.1 Equivalence Relation

One of the deepest analysis of simplex shape measures available is from Liu and Joe [24]. They define the notion of simplex shape measure equivalence in the following way:

Definition 4.1. Let μ and ν be two different simplex shape measures scaled in the interval $[0,\ 1]$. μ and ν are *equivalent* if there exist positive constants c_0, c_1, e_0 and e_1 such that

$$c_0\nu^{e_0} \leq \mu \leq c_1\nu^{e_1}. \tag{4.1}$$

If e_0 (e_1) is the minimum (maximum) possible exponent, then the lower (upper) bound is said *optimal*. If c_0 (c_1) is the maximum (minimum) possible constant, then the lower (upper) bound is said *tight*.

Note that this relation is an equivalence relation for shape measures since it is symmetric, reflexive, and transitive. Indeed, the roles of μ and ν can be reversed in the definition. The symmetry appears as follows: if μ is equivalent to ν with $c_0\nu^{e_0} \leq \mu \leq c_1\nu^{e_1}$, then ν is equivalent to μ with $c_2\mu^{e_2} \leq \nu \leq c_3\mu^{e_3}$, where $c_2 = c_1^{-1/e_1}$, $e_2 = 1/e_1$, $c_3 = c_0^{-1/e_0}$ and $e_3 = 1/e_0$. The transitivity appears as follows: if μ is equivalent to ν with $c_0\nu^{e_0} \leq \mu \leq c_1\nu^{e_1}$ and if ν is equivalent to v with $c_2v^{e_2} \leq \nu \leq c_3v^{e_3}$ then μ is equivalent to v with $c_4v^{e_4} \leq \mu \leq c_5v^{e_5}$, where $c_4 = c_0c_2^{e_0}$, $e_4 = e_0e_2$, $c_5 = c_1c_3^{e_1}$ and $e_5 = e_1e_3$.

4.2 Equivalence of Simplex Shape Measures

Liu and Joe [24] proved the equivalence of the tetrahedron shape measures η, ρ and σ_{min} (Eqs. (2.1), (2.4) and (2.6) respectively). More precisely, they demonstrated the following inequalities with strict upper bounds:

$$
\begin{array}{rr}
\eta^3 \le \rho \le \eta^{3/4}, & \rho^{4/3} \le \eta \le \rho^{1/3}, \\
0.2296\eta^{3/2} \le \sigma_{min} \le 1.1398\eta^{3/4}, & 0.8399\sigma_{min}^{4/3} \le \eta \le 2.6667\sigma_{min}^{2/3}, \\
0.2651\rho^2 \le \sigma_{min} \le \rho^{1/2}, & \sigma_{min}^2 \le \rho \le 1.9420\sigma_{min}^{1/2}.
\end{array}
$$

Furthermore, it can be shown that the η, κ, $\widetilde{\kappa}$ and γ shape measures (Eqs. (2.1), (2.2), (2.3) et (2.7)) belong to the same equivalence relation, at least in two dimensions for γ. Indeed, the following relationship can be verified (the bounds are not necessarily optimal or tight).

$$
\begin{array}{cl}
\frac{2}{3}\gamma^2 \le \rho \le \frac{2}{\sqrt{3}}\gamma & \text{in 2 D}, \\
\kappa^{1/2} \le \widetilde{\kappa} \le d\kappa^{1/2} & \text{in } d \text{ D}, \\
\kappa \le \eta \le d\kappa^{1/d} & \text{in } d \text{ D}, \\
\widetilde{\kappa} \equiv \eta & \text{in 2 D}, \\
\sqrt{2/3}\,\eta^{3/2} \le \widetilde{\kappa} \le 3\eta^{1/2} & \text{in 3 D}.
\end{array}
$$

These equivalence imply that if one of these shape measures approaches zero, which indicates a poorly-shaped simplex, then so do the others. Conversely, if one of these shape measures approaches unity, then so do the others. But the rate at which they approach zero or unity may differ as do μ and $\nu = \mu^2$ for example.

4.3 Equivalence Classes for Shape Measures

The equivalence relation can serve to partition the possible shape measures into equivalence classes. A shape measure would then be equivalent to all shape measures of it's class. In practice, it seems that all the shape measure presented in Sec. 2 belong to the same equivalence class. Indeed, it is the case for η, κ, $\widetilde{\kappa}$, γ, ρ et σ_{min}. It is tempting to conclude that *the equivalence class of Definition 4.1 includes all the shape measures that satisfy Definition 2.1.* But such is not the case. A counter example given by A. Liu serves to prove this point.

Let μ be a shape measure that satisfy Definition 2.1, then $\nu = 2^{(\mu-1)/\mu}$ is also a shape measure according to Definition 2.1. It can not be proven that μ et ν are equivalent according to Definition 4.1 since there does not exist any constants c_0 and e_0 such that $c_0\mu^{e_o} \le \nu$ when μ tends toward zero. This is due to the fact that the exponential asymptotic behavior of ν tends towards zero faster than any possible polynomial asymptotic behavior.

Although the equivalence relation is weak, it is still possible to compare meshes obtained by optimizing different shape measures. Indeed, any shape measures that satisfy Definition 2.1 can be used by a mesh optimizer. Remember that, by definition, they will all detect all simplex degeneracies. They will all be sensitive to badly shaped simplices. Moreover, the more a mesh is optimized with a given simplex shape measure, the closer to the optimal mesh it is for any other simplex shape measure. In the limit, if it were possible to mesh a domain with only equilateral simplicies, as it is in two dimensions, all mesh optimizers should converge to that mesh, whatever shape measure is used in the mesh optimizer. These assertions are justified in the next section.

4.4 Practical comparison of shape measures

Three two-dimensional test-cases are presented to practically compare various shape measures. Due to the problem of visualizing tetrahedral meshes, no three-dimensional example is given. Results can be extended to the third dimension except that no perfect mesh exists in three dimensions. It is impossible to fill space with regular tetrahedra. So, the optimal mesh is always unknown and slightly depends on the tetrahedron shape measure used.

The test-cases are optimized using the mesh optimization package **OO**$\mathcal{RT}$(Object-Oriented Remeshing Toolkit)[1]. It can be described as a mesh optimizer that acts on every characteristics of a mesh, namely the number of vertices, vertex coordinates and simplex connectivity. It is based on an algorithm performing successive local modifications such as mesh refinement, edge collapsing, vertex relocation or vertex reconnection. Stopping criteria are tight enough to perform a real mesh optimization, not only mesh enhancement.

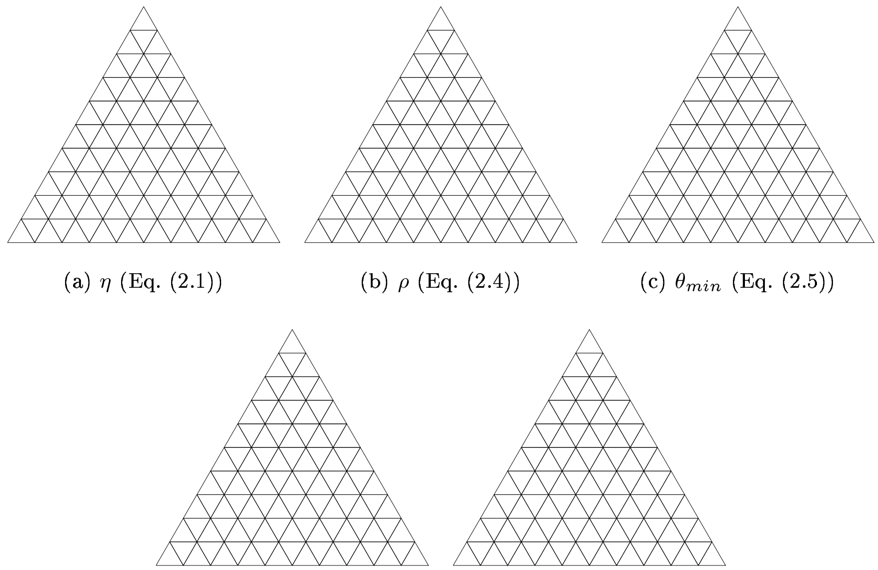
In two dimensions, for certain domains, a perfect mesh can be obtained in which all the triangles are optimal. For instance, the domain consisting of an equilateral triangle meshed using an uniform target size of $1/10$ of the domain edge length can be meshed using only equilateral triangles. In that case, the initial mesh has no influence on the result since it is unique. Using the same algorithm with various shape measures, the perfect mesh must be obtained, and is obtained with the mesh optimizer.

This example shows that the triangle shape measure has no effect on the final mesh, if a perfect mesh can be obtained. If the heuristic used by the mesh optimizer is able to get it, it will obtain it, whatever shape measure is used. In this example, three measures have led to exactly the same choices during the whole process: the same 124 edges have been swapped, on about 2000 checked edges. The values of the shape measures differed but comparing the same configurations drove to the same decisions.

The previous example is really academic since perfect meshes are impossible on almost every domain. The next example is a square. Optimal meshes are not perfect, so they vary with the shape measure. But differences are small (see Fig. 7). The choice of a shape measure has more effect when the optimal mesh is far from a perfect mesh.

The last test-case is the same as the first one, but the optimization algorithm differs. Vertex relocation has been excluded from the possible mesh modifications. The resulting optimizer is less powerful, so it is not surprising that the final meshes are not perfect anymore (Fig. 8).

[1] See `http://www.cerca.umontreal.ca/oort.`



(a) η (Eq. (2.1)) (b) ρ (Eq. (2.4)) (c) θ_{min} (Eq. (2.5))

(d) γ (Eq. (2.7)) (e) r (Eq. (2.9))

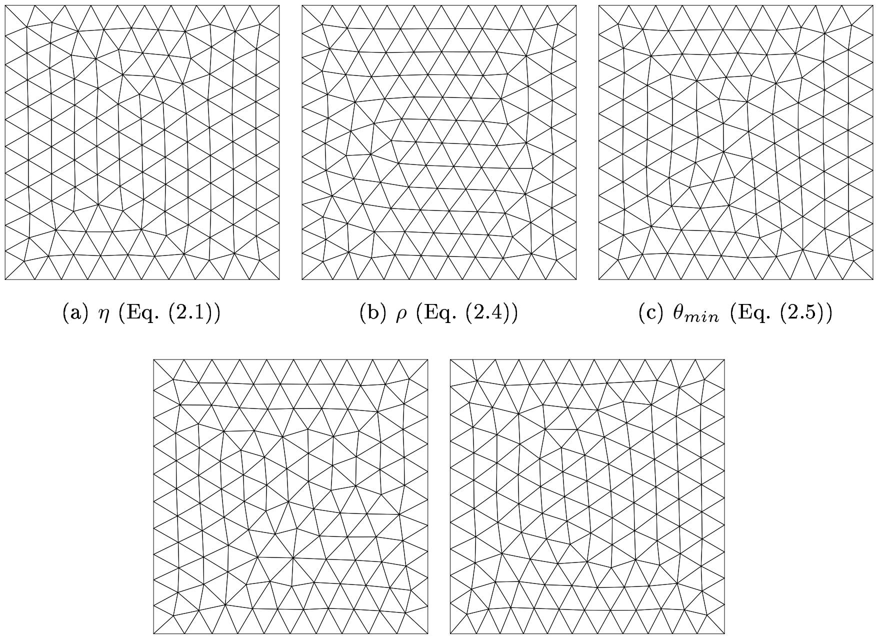
Figure 6: Simplex meshes of an equilateral triangular domain with a mesh target edge length of 1/10 of the domain size and with five different triangle shape measures.

Although the five meshes obtained from various shape measures differ significantly, it is not right to conclude from these differences that one shape measure is better than the other. The only valid conclusion is that the mesh optimizer is not powerful enough to reach the optimal mesh. The problem is in the optimization algorithm, not in the simplex shape measure used for optimization.

Conclusions

A taxonomy of simplex degeneracies has been proposed and a systematic way of classifying them based on the final configuration of the degenerate simplex is presented in tables. A definition of simplex shape measure has been put forth that takes into account all possible degeneracies. Using this definition, commonly used shape measures were cast into a standard notation and analyzed to determine which were valid shape measures. A method was given to use them for anisotropic meshing by extending the shape measures to Riemannian space by expressing basic concepts such as length, area and volume in a metric.

Several shape measures were visually compared which has clearly expressed the regularity of the mean ratio η (Eq. (2.1)) and the radius ratio ρ (Eq. (2.4)), and the shortcomings of invalid shape measures were particularly



(a) η (Eq. (2.1)) (b) ρ (Eq. (2.4)) (c) θ_{min} (Eq. (2.5))

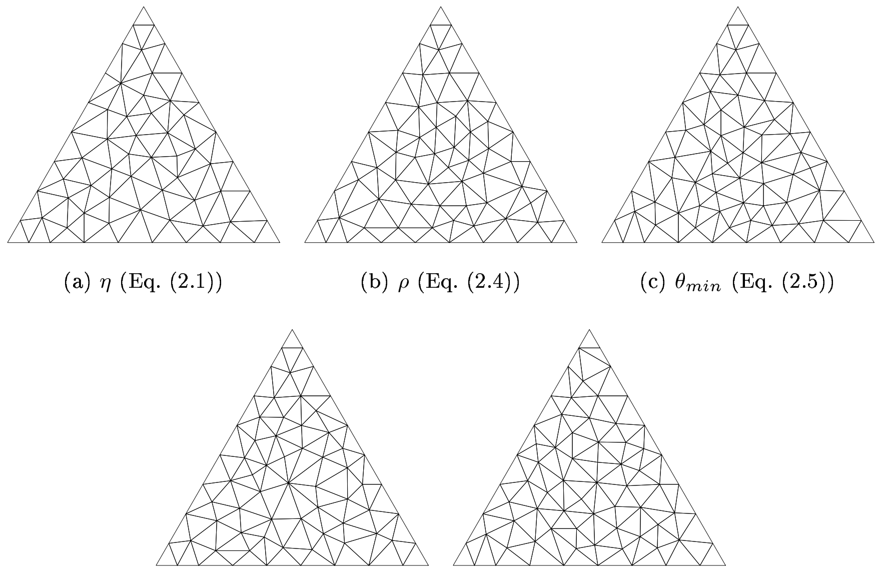
(d) γ (Eq. (2.7)) (e) r (Eq. (2.9))

Figure 7: Simplex meshes of a square domain with a mesh target edge length of 1/10 of the domain size, using five different triangle shape measures.

evident. All the commonly used shape measures were then compared using the equivalence relation of Liu and Joe [24], and all were shown to be in the same equivalence class. Furthermore, it was shown on academic test-cases that the choice of a shape measure to drive mesh optimization is much less crucial that the power of the mesh optimizer.

Although all of the tested shape measures yielded comparable results, the mean ratio η (Eq. (2.1)) is particularly appealing due to its simplicity and its regularity.

From the present work, it can be concluded that more attention should be given to optimization and generation algorithms rather than defining new shape measures. Indeed, *our intuition* about mesh generation and optimization is that it is a *non linear*, and even *discontinuous* problem. It is therefore impossible to generate directly the optimal mesh. The optimal mesh can only be reached with an iterative process that can remove vertices, change the coordinates of the vertices and change the connectivity between vertices. These are the operations that allow to handle all degrees of freedom of a mesh. All these operations must be combined together in an heuristic such that they work together in the same direction and that they converge towards the optimal mesh. Ideally, they should optimize the same objective function measuring how much a mesh fits



(a) η (Eq. (2.1))

(b) ρ (Eq. (2.4))

(c) θ_{min} (Eq. (2.5))

(d) γ (Eq. (2.7))

(e) r (Eq. (2.9))

Figure 8: Simplex meshes of an equilateral triangular domain with the same target and the same triangle shape measures as on Fig. 6. Only the optimization algorithm differs.

with the target. In that context, the choice of a specific shape measure has far less impact on the final mesh than the careful combination of operations within the optimization strategy.

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A Notion of Riemannian Metric

The standard way of measuring distances in Euclidean space is a special case of a more general approach to measure that shall be briefly summarized here. The objective behind the introduction of this length measurement approach is to recast in a more general framework the various numerical constraints imposed by applications on numerical mesh generation and adaptation. Each type of application imposes domain specific constraints on mesh generation in terms of optimal element size distribution, element size distortion and stretching. Through the use of a metric, constraints can be expressed in domain independent terms, and in doing so, mesh quality can be assessed in absolute terms, regardless of specific application domains.

In order to abstract shape and size specifications, which can take numerous forms and names, a general tensorial approach is taken, whereby all desired mesh characteristics are expressed in terms of a continuous second order tensor. The Riemannian metric framework was chosen for mesh constraints representation since this formalism can account for both isotropic and anisotropic mesh control specifications, and includes a wide range of size and shape specification schemes in current use in the literature.

Let P be a point in space $\mathbb{R}^d$, and $\mathcal{M}(P)$ be a continuous second order symmetric tensor field define over $\mathbb{R}^d$. If $\mathcal{M}(P)$ is symmetric positive definite, it can be expressed as the product of three tensors:

$$\mathcal{M}(P) = R^T(P)\, D(P)\, R(P), \tag{A.1}$$

with $R(P)$ a rotation tensor, $R^T(P) = R^{-1}(P)$ the inverse rotation tensor, and $D(P)$ a diagonal tensor with all terms strictly positive. These diagonal terms are the eigenvalues of $\mathcal{M}(P)$. The metric tensor field $\mathcal{M}(P)$ associated with a method to measure distance then defines a *Riemannian metric* or simply a *metric* over space $\mathbb{R}^d$.

A.1 Length

With this definition, many simplex quantities can be rewritten in terms of the metric. First, the length of a parametric curve $\gamma(t) = \{(x(t), y(t), z(t)),\, t \in [0,1]\}$ can be expressed in metric space $\mathcal{M}$ by equation

$$L_{\mathcal{M}}(\gamma) = \int_0^1 \sqrt{(\gamma'(t))^T\, \mathcal{M}\, (\gamma(t))\ \gamma'(t)}\, dt. \tag{A.2}$$

In this expression, $\gamma(t)$ represents a point on the curve and $\gamma'(t)$ the tangent vector at that point.

Mavriplis [29] introduced metric change in terms of local space deformation. To illustrate this, lets denote

$$D = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix},$$

the diagonal tensor made up of the eigenvalues of the metric tensor in 3-space. The local linear transformation N

$$N = \begin{pmatrix} \sqrt{\lambda_1} & 0 & 0 \\ 0 & \sqrt{\lambda_2} & 0 \\ 0 & 0 & \sqrt{\lambda_3} \end{pmatrix} R, \tag{A.3}$$

can now be constructed from $R(P)$, the rotation tensor, and $D^{1/2}$. This local transformation relates to the metric $\mathcal{M}$ in the way that it is equivalent to measure the length of a vector X in the original space through the metric $\mathcal{M}$, or to measure the length of the transformed vector $N\,X$. Indeed,

$$X^T\,\mathcal{M}\,X = X^T\,N^T\,N\,X = (N\,X)^T\,N\,X = \|N\,X\|^2, \tag{A.4}$$

Lengths are thus easily measured with a metric. Shape measures, however, are often expressed in terms not only of lengths, but also of area, volume and angles, which must also be computed using a metric.

A.2 Measure

The measure of simplex K — area in two dimensions and volume in three dimensions — in the metric $\mathcal{M}$, is the integral of the square root of the metric's determinant over K. This measure will be denoted $V_K^{\mathcal{M}}$. Through a change of variable, using Eq. A.4, we can write

$$V_K^{\mathcal{M}} = \int_{N(K)} 1\, dV = \int_K \det(N)\, dV$$

since $\det(N)$ is the Jacobian of the linear transformation. Moreover, from Eq. (A.3), we have $\det(\mathcal{M}) = (\det(N))^2$, so that

$$V_K^{\mathcal{M}} = \int_K \sqrt{\det(\mathcal{M})}\, dV. \tag{A.5}$$

This integral can be computed numerically using a quadrature rule. Approximate formulae can also be derived, that are based on edge lengths, as are presented in the following appendices.

A.3 Angle

Another quantity often involved in shape measure is the angle between two vectors in the metric space. Let two vectors V and W that meet at point P, we have

$$\cos(\theta) = \frac{V^T \mathcal{M}(P)\, W}{\|N\, V\| \cdot \|N\, W\|} \tag{A.6}$$

where θ is the angle between V and W.

B Approximate Formulae for the Triangle

When dealing with shape measures in metric space, computation of all quantities must be recast in this new framework. While some basic quantities can be precisely expressed and numerically computed using exact maths, derived quantities tend to become very involved in terms of computational complexity and cost. For that reason, approximate formulae are often very helpful to help analyze and compare shape measures in metric space. The following formulae are valid in Euclidean and for uniform metric spaces. A uniform metric space is a deformed space where the deformation tensor is constant from point to point.

Since edge length is the simplest measure to compute over a simplex, care has been taken to formulate all these approximate formulae in terms of edge lengths measured in Euclidean or metric space.

Let K stands for a non degenerate triangle with vertices P_1, P_2 and P_3; S_K denotes the area of K and $L_{ij} = \|P_j - P_i\|, 1 \leq i < j \leq 3$, denotes the length of the three edges $\overline{P_i P_j}$ of K.

The half-perimeter p_K, the inradius ρ_K and the circumradius r_K are given by

$$p_K = \frac{(L_{12} + L_{13} + L_{23})}{2}, \qquad \rho_K = \frac{S_K}{p_K}, \qquad r_K = \frac{L_{12}\, L_{13}\, L_{23}}{4 S_K}. \tag{B.1}$$

In finite elements terms, the diameter h_{max} of an element is the maximum Euclidean distance between two points of an element, which is the longest edge for a simplex. The smallest edge of an element is denoted h_{min}.

$$h_{max} = \max(L_{12}, L_{13}, L_{23}), \qquad h_{min} = \min(L_{12}, L_{13}, L_{23}). \tag{B.2}$$

The angle θ_i at vertex P_i of the triangle K is expressed as a function of the edge lengths as

$$\theta_i = \arcsin\left(2 S_K \left(\prod_{\substack{j,k \neq i \\ 1 \leq j < k \leq 3}} L_{ij} L_{ik} \right)^{-1} \right). \tag{B.3}$$

Finally, the area S_K of the triangle can also be expressed as a function of its edge lengths by Heron's formula:

$$S_K^2 = p_K(p_K - L_{12})(p_K - L_{13})(p_K - L_{23}). \tag{B.4}$$

Note that if the three lengths used, L_{12}, L_{13} and L_{23}, do not form a triangle, i.e. they do not satisfy the triangular inequality, as it can happen in a non-Euclidean metric, then the square of the area has a negative value. Heron's formula has no sense in that case. One must then resort to Eq. A.5 in order to compute the precise triangular area in metric space.

C Approximate Formulae for the Tetrahedron

As for the triangle, the knowledge of the edge lengths of a tetrahedron is sufficient to uniquely define a tetrahedron in Euclidean or constant metric space. Significant formulae for the tetrahedron can thus be expressed in terms of its edge lengths, which will be valid, again, if sharp deformations in space are not encompassed in single mesh elements.

Let K stands for a non degenerate tetrahedron with vertices P_1, P_2, P_3 and P_4; $L_{ij} = \|P_j - P_i\|, 1 \leq i < j \leq 4$, denotes the length of the six edges $\overline{P_iP_j}$ of K; S_1 denotes the area of the triangular face $\triangle P_2P_3P_4$, S_2 the area of face $\triangle P_1P_3P_4$, S_3 the area of face $\triangle P_1P_2P_4$ and S_4 the area of face $\triangle P_1P_2P_3$; V_K denotes the volume of tetrahedron K.

The inradius ρ_K and the circumradius r_K are given by

$$\rho_K = \frac{3V_K}{S_1 + S_2 + S_3 + S_4},$$

$$r_K = \frac{\sqrt{(a+b+c)(a+b-c)(a+c-b)(b+c-a)}}{24V_K}, \tag{C.2}$$

where $a = L_{12}L_{34}$, $b = L_{13}L_{24}$ and $c = L_{14}L_{23}$ are the products of opposite edge lengths of K. In a tetrahedron, two edges are opposed if they share no vertices.

The minimum and maximum edge lengths h_{min} and h_{max} are trivially given by

$$h_{min} = \min(L_{12}, L_{13}, L_{14}, L_{23}, L_{24}, L_{34}), \qquad h_{max} = \max(L_{12}, L_{13}, L_{14}, L_{23}, L_{24}, L_{34}). \tag{C.3}$$

The solid angle θ_i at the vertex P_i of the tetrahedron is defined to be the surface area formed by projecting each point of the face not containing P_i to the unit sphere centered at P_i. Liu and Joe [24] give a formula to compute solid angles of a tetrahedron in terms of edge lengths

$$\theta_i = 2 \arcsin\left(12V_K \left(\prod_{\substack{j,k \neq i \\ 1 \leq j < k \leq 4}} \left((L_{ij} + L_{ik})^2 - L_{jk}^2 \right) \right)^{-1/2} \right). \tag{C.4}$$

Finally, the volume V_K of a tetrahedron can also be expressed as a function of its edge lengths. Let a, b, c, e, f and g, the length of the six edges of the tetrahedron. Edges a, b and c connect to the same vertex of the tetrahedron, e is the edge opposite of a, f to b and g to c. The edges e, f and g are the three sides of a face of the tetrahedron, opposite to the vertex to which a, b and c connect. For example, a, b, c, e, f and g can be L_{12}, L_{13}, L_{14}, L_{34}, L_{24} and L_{23} respectively. Then, the volume of the tetrahedron is given by [31]

$$\begin{aligned} 144V_K^2 &= 4a^2b^2c^2 + \left(b^2+c^2-e^2\right)\left(c^2+a^2-f^2\right)\left(a^2+b^2-g^2\right) \\ &- a^2\left(b^2+c^2-e^2\right) - b^2\left(c^2+a^2-f^2\right) - c^2\left(a^2+b^2-g^2\right). \end{aligned} \quad \text{(C.5)}$$

Contrary to Heron's formula (B.4) in two dimensions, this three-dimensional version of Heron's formula is not symmetric. The three edges a, b and c which start from the same vertex do not play the same role as the three edges e, f and g which share a face. Eq. (C.5) can be rewritten in a formula that exhibits more symmetry [31]. However, it is costlier to compute and more subject to roundoff error.

Note that if the six lengths do not form a tetrahedron, as can happen in a non-Euclidean metric, then the square of the volume has a negative value. Heron's three-dimensional formula has no sense in that case. One must then resort to Eq. A.5 in order to compute the precise tetrahedral volume in metric space.